

Chlorhexidine

55-56-1 | DTXSID2033314

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 318 °C

Global applicability domain: Outside

Local applicability domain index: 3.23e-02

Confidence level: 3.93e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Aminotrimethylene phosphonic acid</div> <div>Measured: 480</div> <div>Predicted: 478</div>	<div>Image not found</div> <div>Diphenylurea</div> <div>Measured: 262</div> <div>Predicted: 269</div>	<div>Image not found</div> <div>N-(4-Bromophenyl)urea</div> <div>Measured: 260</div> <div>Predicted: 256</div>
<div>Image not found</div> <div>1-Phenylurea</div> <div>Measured: 238</div> <div>Predicted: 247</div>	<div>Image not found</div> <div>Tetraethylenepentamine</div> <div>Measured: 342</div> <div>Predicted: 339</div>	